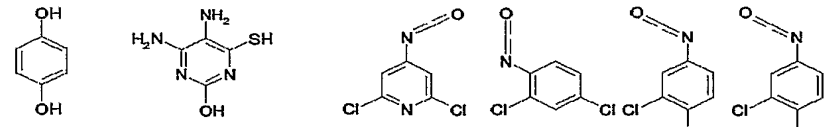
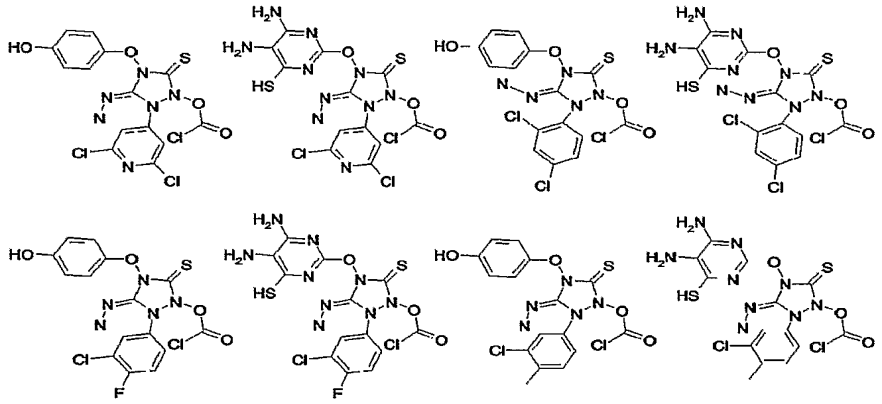
Figure 1

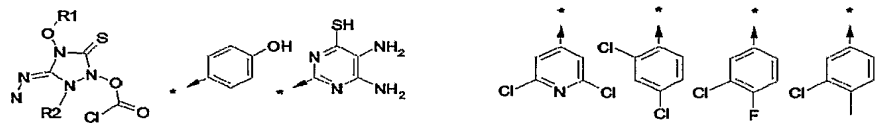


Chemicals of set R1 Chemicals of set R2

Under certain conditions, each chemical in set R1 may react with each chemical in set R2 and yield to the following set of compounds:



These eight compounds are represented by the following non-enumerated library. This representation is also called Markush representation:



Library scaffold Set R1 Set R2

The Markush representation

Figure 2

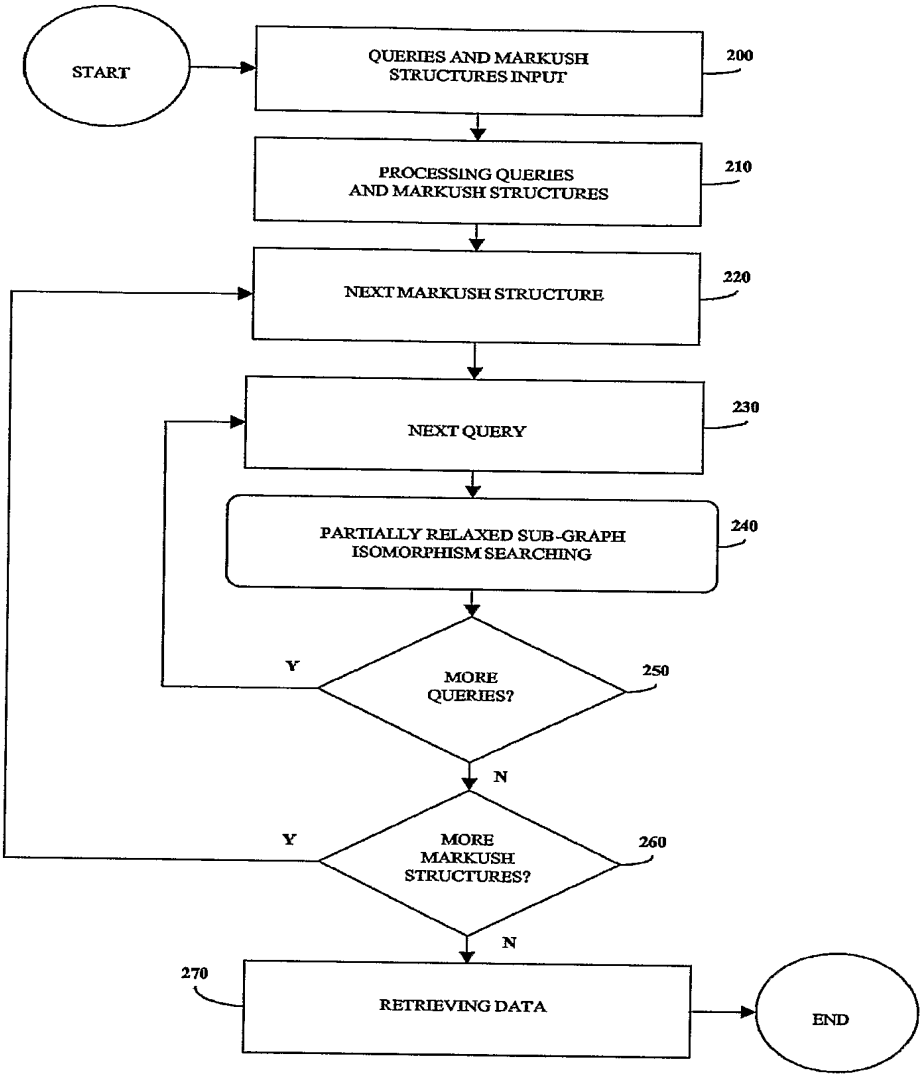

START
QUERIES AND MARKUSH STRUCTURES INPUT
200
PROCESSING QUERIES AND MARKUSH STRUCTURES
210
NEXT MARKUSH STRUCTURE
220
NEXT QUERY
230
PARTIALLY RELAXED SUB-GRAPH ISOMORPHISM SEARCHING
240
MORE QUERIES?
250
Y
N
MORE MARKUSH STRUCTURES?
260
Y
N
270
RETRIEVING DATA
END

Figure 3

SUBROUTINE:
PARTIALLY RELAXED SUB-GRAPH ISOMORPHISM SEARCHING

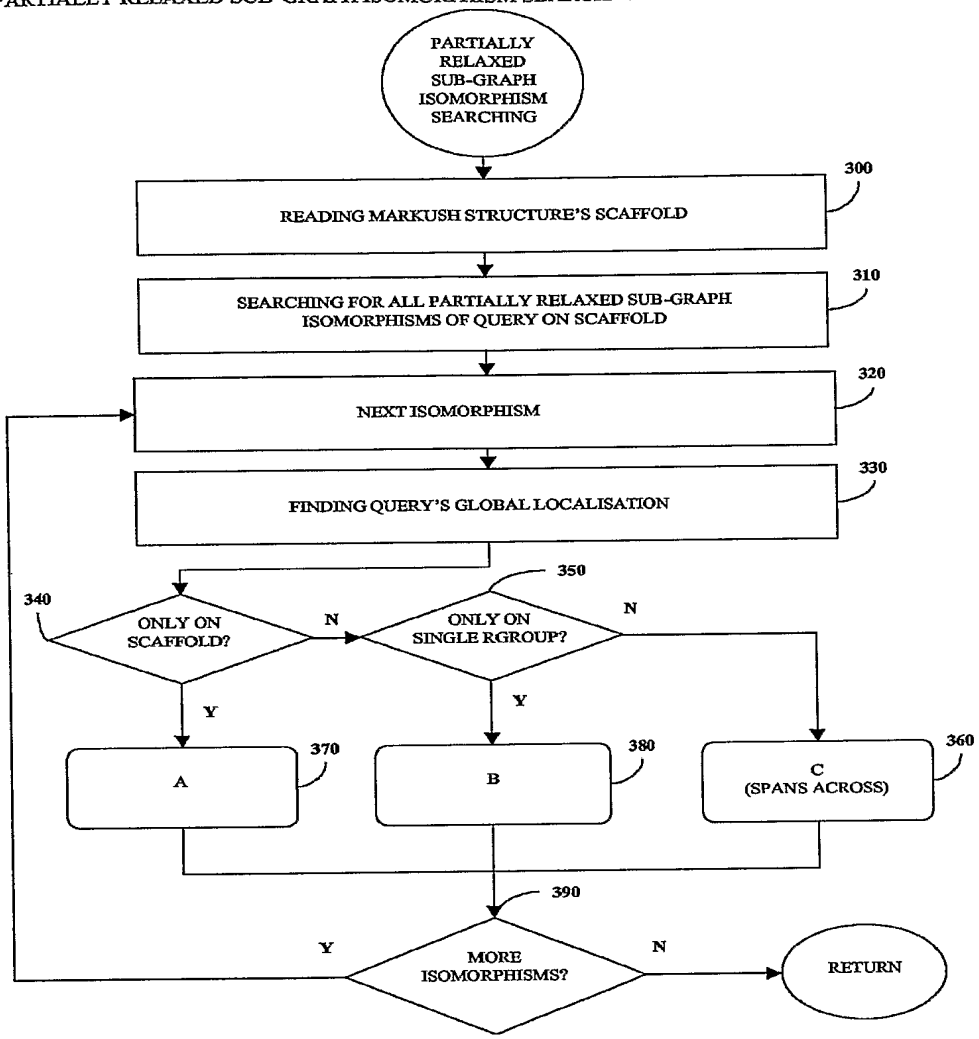


Figure 4

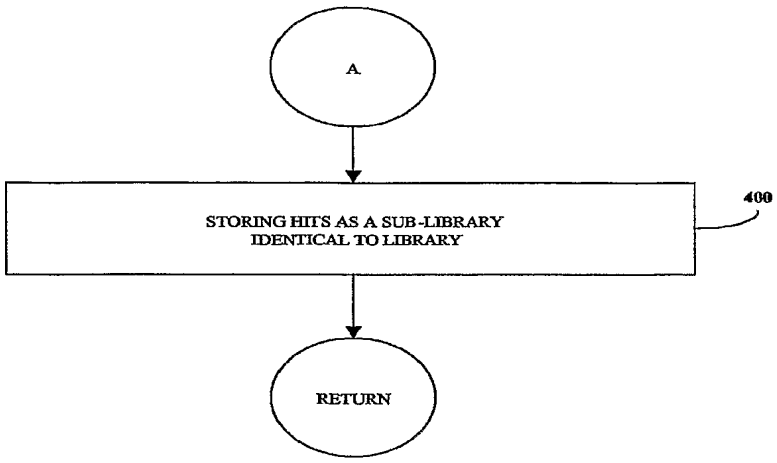

SUBROUTINE:
A (QUERY IS LOCATED ONLY ON THE SCAFFOLD)
A
STORING HITS AS A SUB-LIBRARY
IDENTICAL TO LIBRARY
400
RETURN

Figure 5

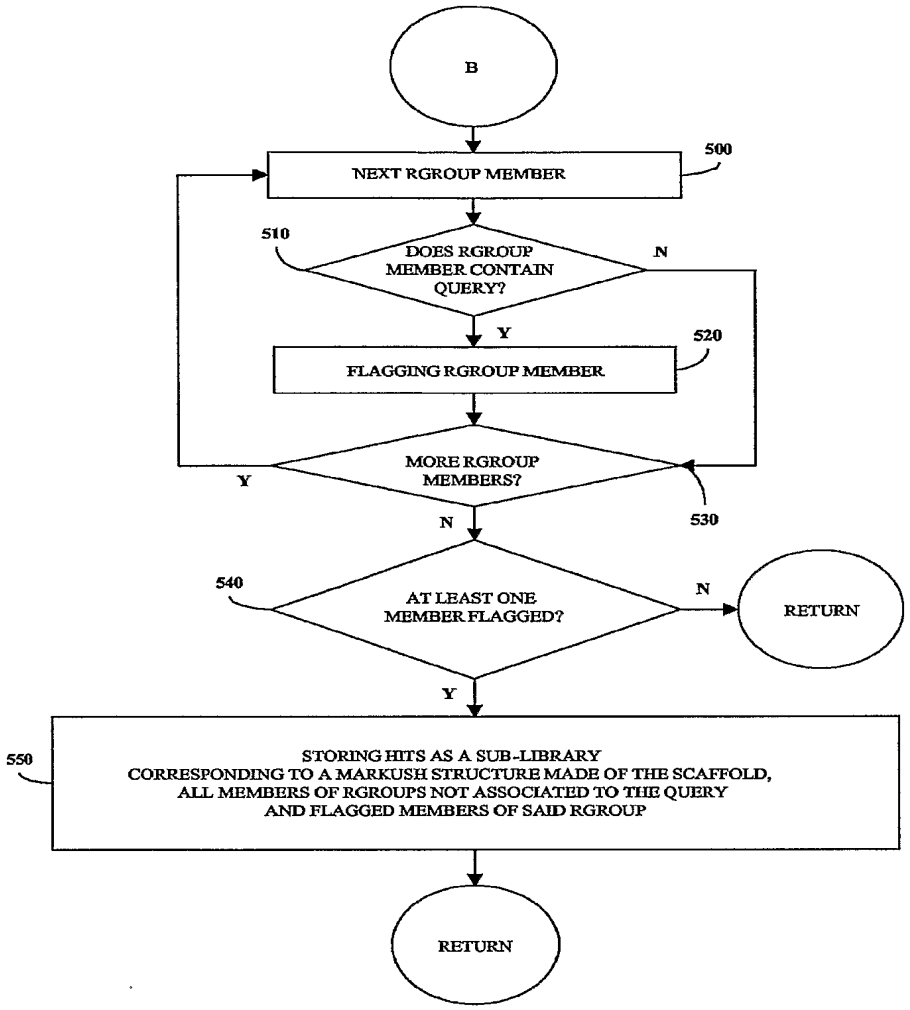

SUBROUTINE:
B (QUERY IS LOCATED ONLY ON A SINGLE RGROUP)
B
NEXT RGROUP MEMBER
500
510
DOES RGROUP MEMBER CONTAIN QUERY?
N
Y
520
FLAGGING RGROUP MEMBER
MORE RGROUP MEMBERS?
Y
N
530
540
AT LEAST ONE MEMBER FLAGGED?
N
RETURN
Y
550
STORING HITS AS A SUB-LIBRARY CORRESPONDING TO A MARKUSH STRUCTURE MADE OF THE SCAFFOLD, ALL MEMBERS OF RGROUPS NOT ASSOCIATED TO THE QUERY AND FLAGGED MEMBERS OF SAID RGROUP
RETURN

Figure 6

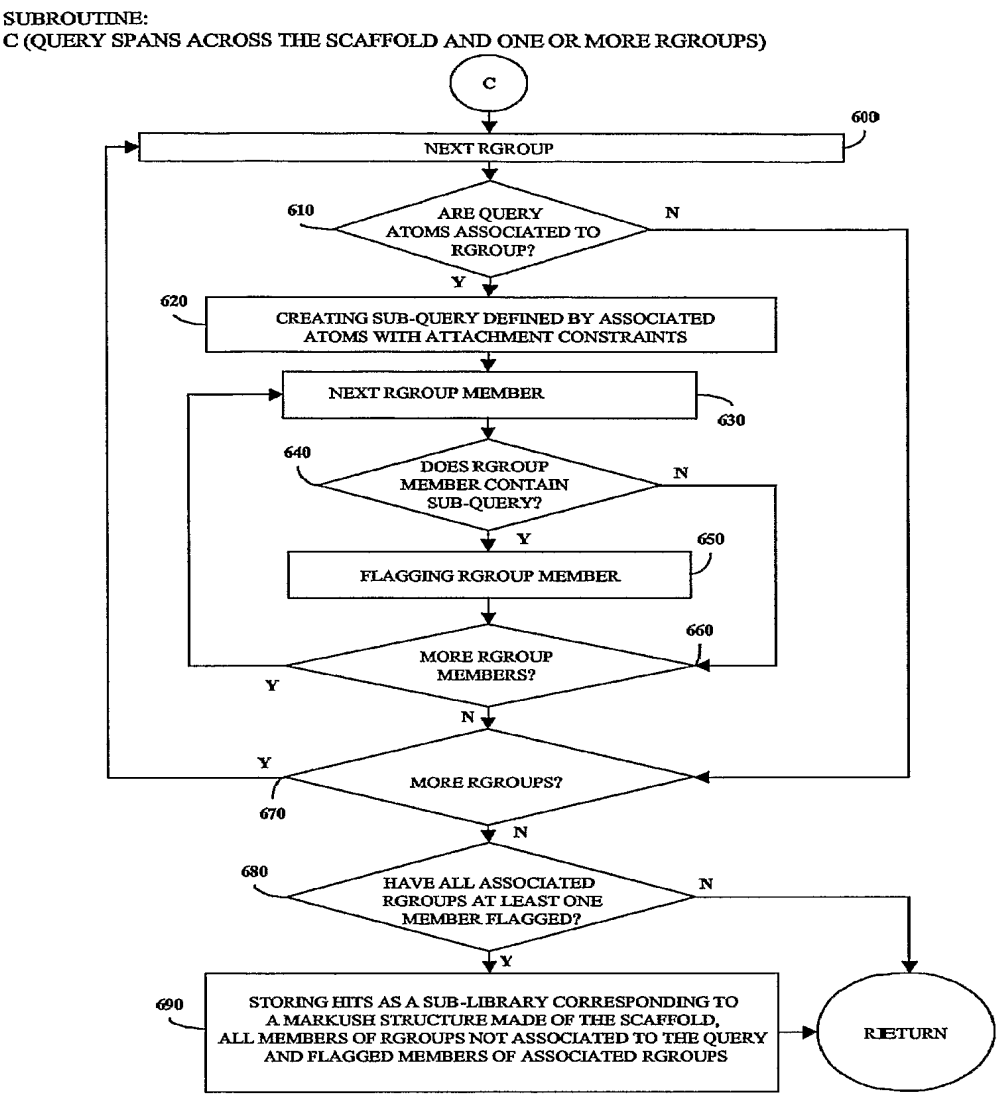

SUBROUTINE:
C (QUERY SPANS ACROSS THE SCAFFOLD AND ONE OR MORE RGROUPS)
C
600
NEXT RGROUP
610
ARE QUERY ATOMS ASSOCIATED TO RGROUP?
N
Y
620
CREATING SUB-QUERY DEFINED BY ASSOCIATED ATOMS WITH ATTACHMENT CONSTRAINTS
NEXT RGROUP MEMBER
630
640
DOES RGROUP MEMBER CONTAIN SUB-QUERY?
N
Y
650
FLAGGING RGROUP MEMBER
660
MORE RGROUP MEMBERS?
Y
N
Y
MORE RGROUPS?
670
N
680
HAVE ALL ASSOCIATED RGROUPS AT LEAST ONE MEMBER FLAGGED?
N
Y
690
STORING HITS AS A SUB-LIBRARY CORRESPONDING TO A MARKUSH STRUCTURE MADE OF THE SCAFFOLD, ALL MEMBERS OF RGROUPS NOT ASSOCIATED TO THE QUERY AND FLAGGED MEMBERS OF ASSOCIATED RGROUPS
RETURN

Figure 7

TEST USED IN SUBROUTINES B AND C
DOES RGROUP MEMBER CONTAIN QUERY OR SUB-QUERY?

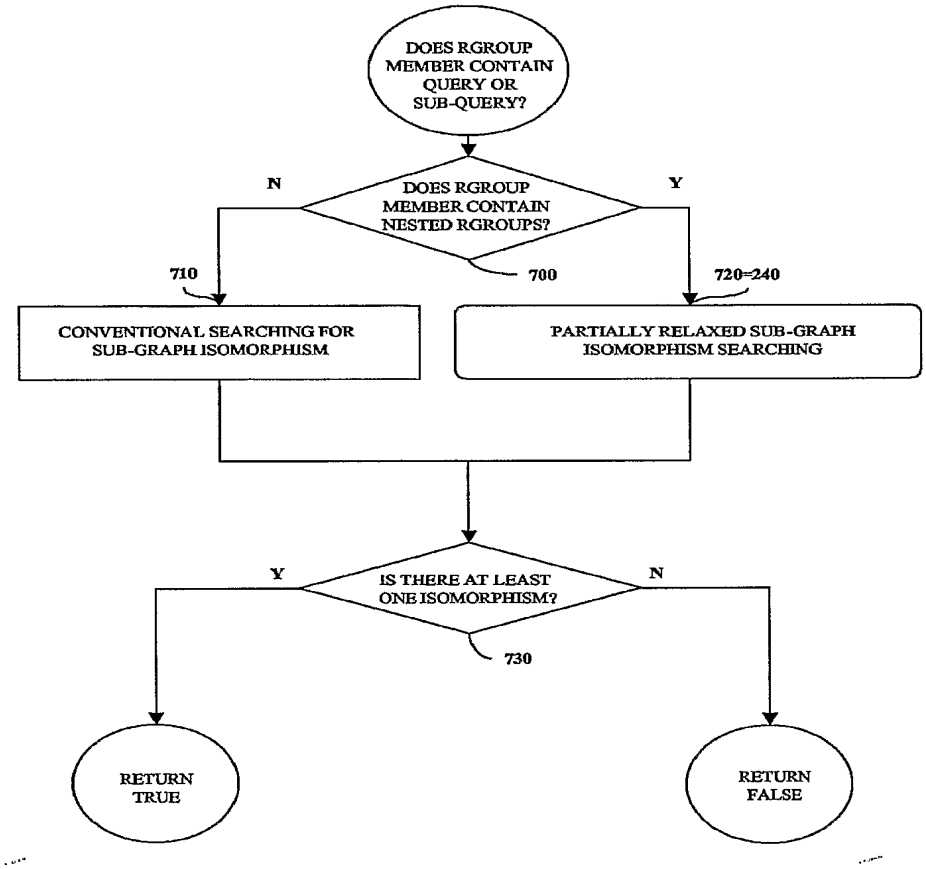
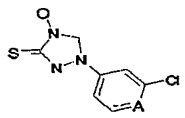
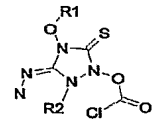


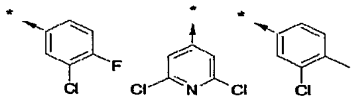
Figure 8



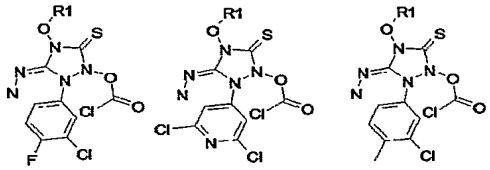
Query structure



Library scaffold



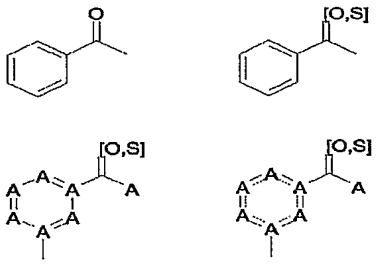
Hits in set R2



Corresponding enumerated hits

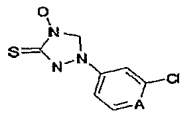
Example of search

Figure 9

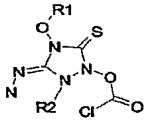


Examples of query structures handled by the method

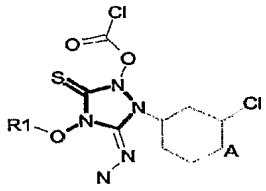
Figure 10



Query structure



Library scaffold



Example of localization

Example of query structure localization

Figure 11

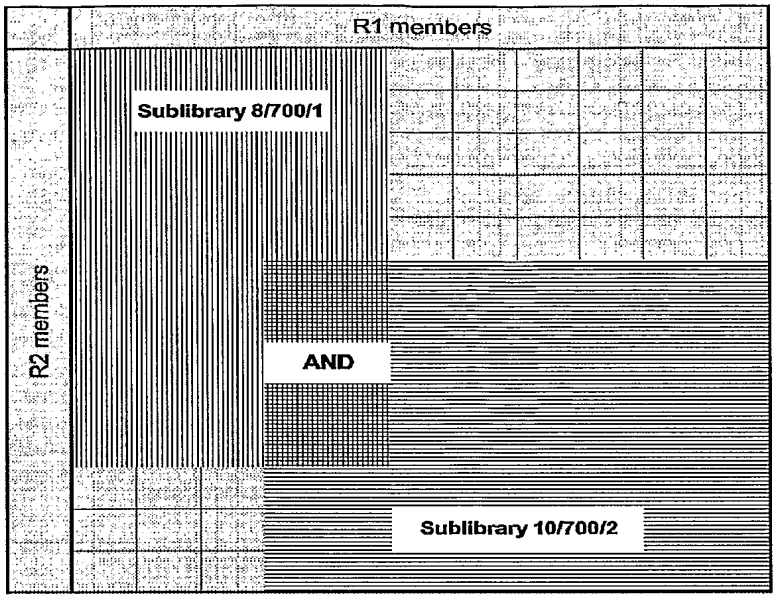
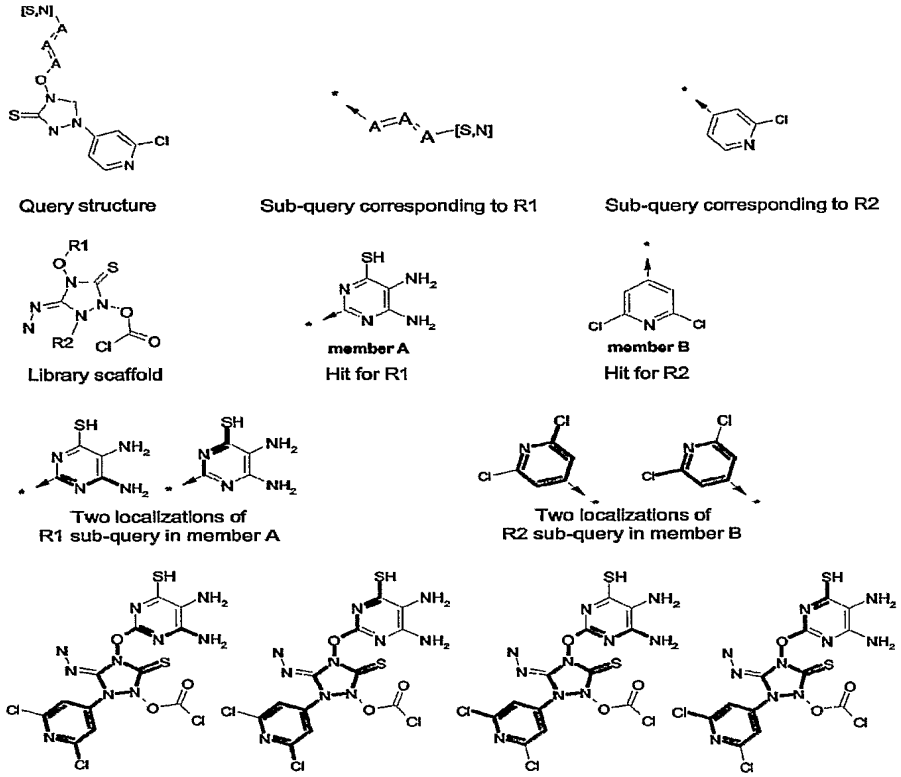

R1 members
Sublibrary 8/700/1
R2 members
AND
Sublibrary 10/700/2

Figure 12



Counting the occurence of a query structure in compounds for a given isomorphism

Figure 13

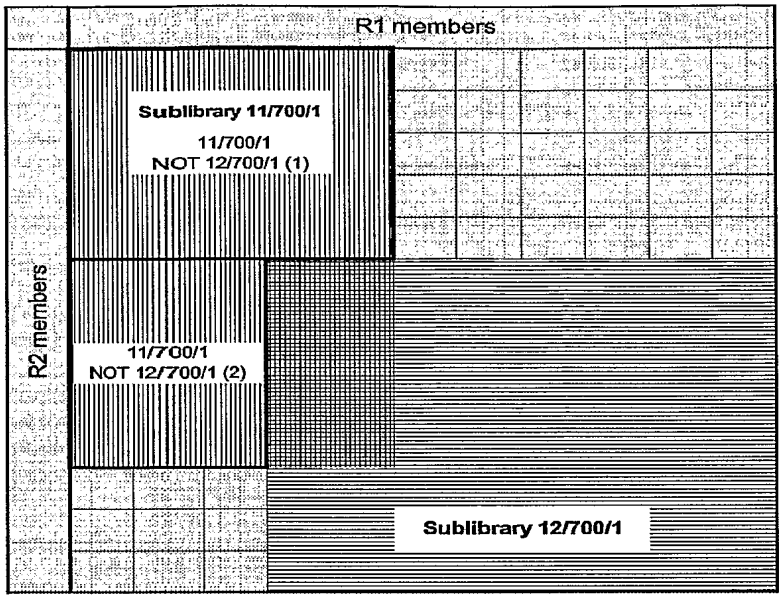

R1 members
Sublibrary 11/700/1
11/700/1
NOT 12/700/1 (1)
R2 members
11/700/1
NOT 12/700/1 (2)
Sublibrary 12/700/1

Figure 14

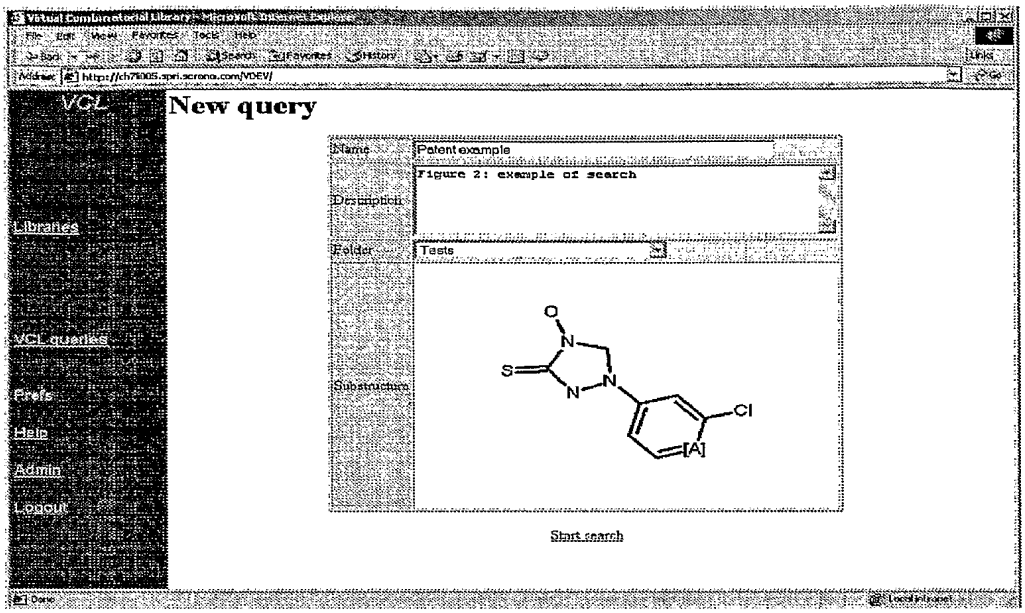

VCL
New query
Libraries
VCL queries
Prefs
Help
Admin
Logout
Name
Patent example
Description
Figure 2: example of search
Folder
Tests
Substructure
O
N
S
N
N
Cl
[A]
Start search

Figure 15

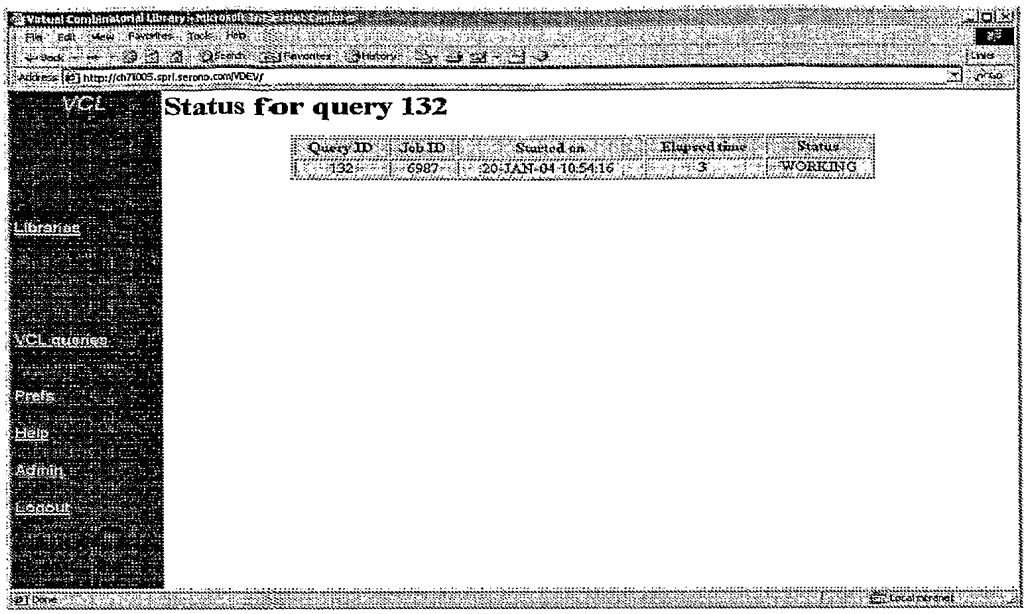

Status for query 132
Query ID
Job ID
Started on
Elapsed time
Status
132
6987
20-JAN-04 10.54.16
3
WORKING
Libraries
VCL queries
Prefs
Help
Admin
Logout

Figure 16

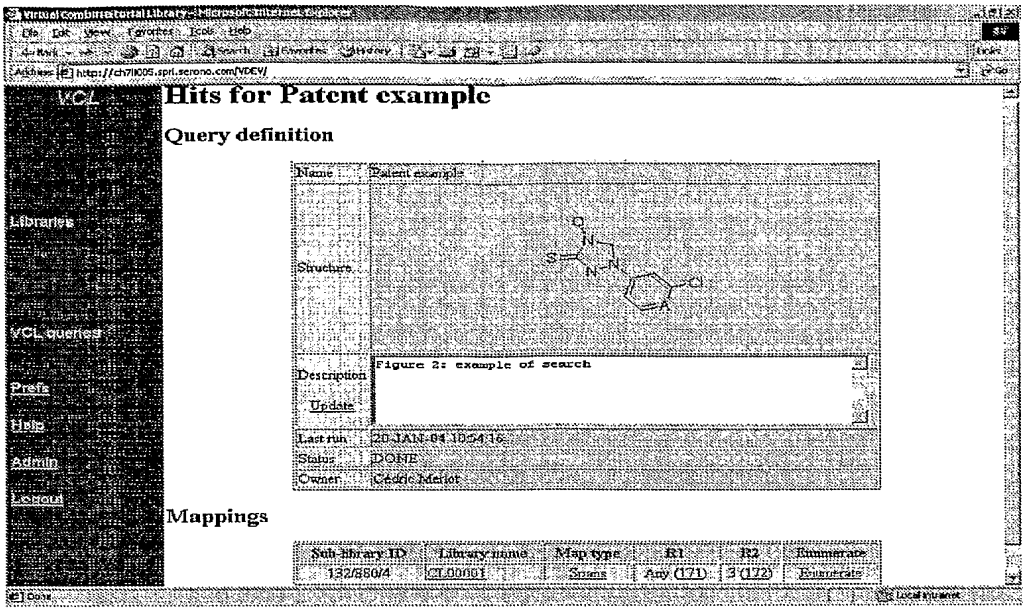

VCL
Libraries
VCL queries
Prefs
Help
Admin
Logout
Hits for Patent example
Query definition
Name
Patent example
Structure
Description
Figure 2: example of search
Update
Last run
20-JAN-04 10:54:16
Status
DONE
Owner
Cédric Mériot
Mappings
Sub-library ID
Library name
Map type
R1
R2
Enumerate
132/880/4
CT-00001
Seven
Any (171)
3 (172)
Enumerate

Figure 17

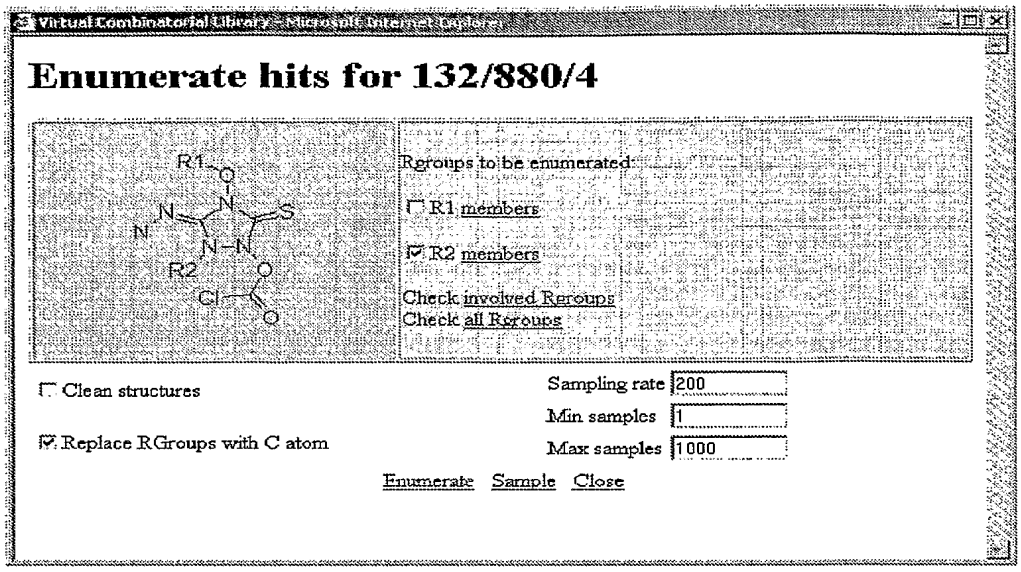

Virtual Combinatorial Library - Microsoft Internet Explorer
Enumerate hits for 132/880/4
R1
O
N
N
S
N
N
N
R2
O
Cl
O
Rgroups to be enumerated:
R1 members
R2 members
Check involved Rgroups
Check all Rgroups
Clean structures
Replace RGroups with C atom
Sampling rate 200
Min samples 1
Max samples 1000
Enumerate Sample Close

Figure 18

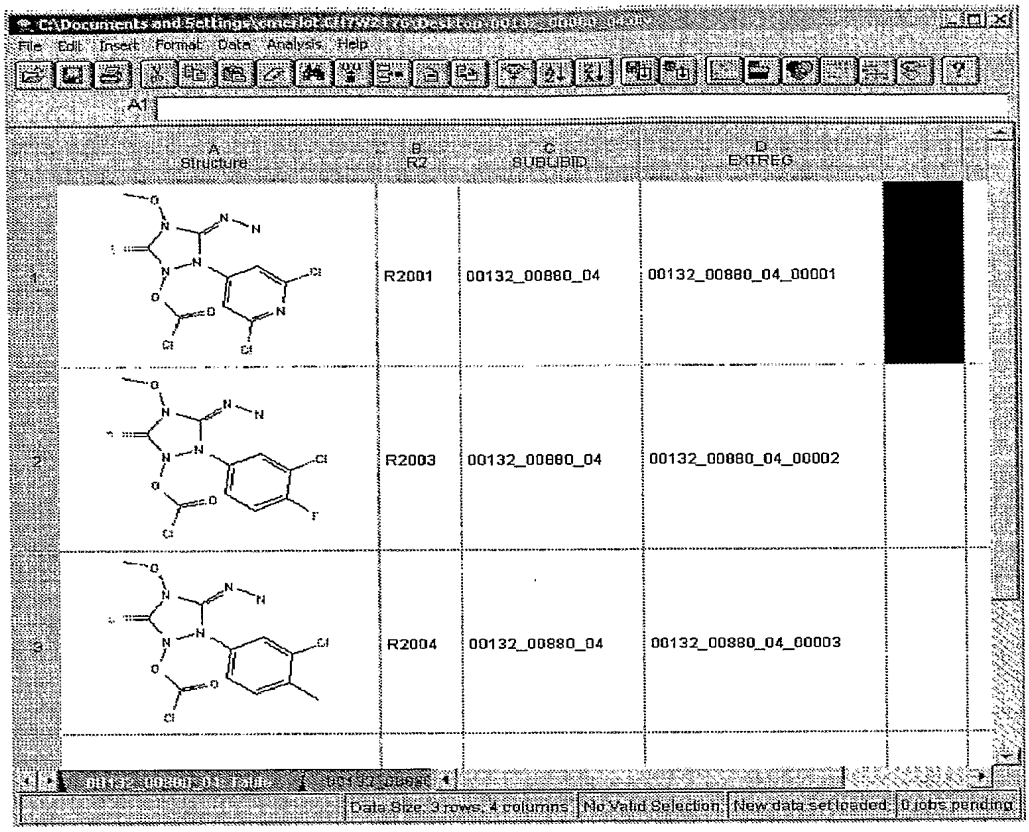
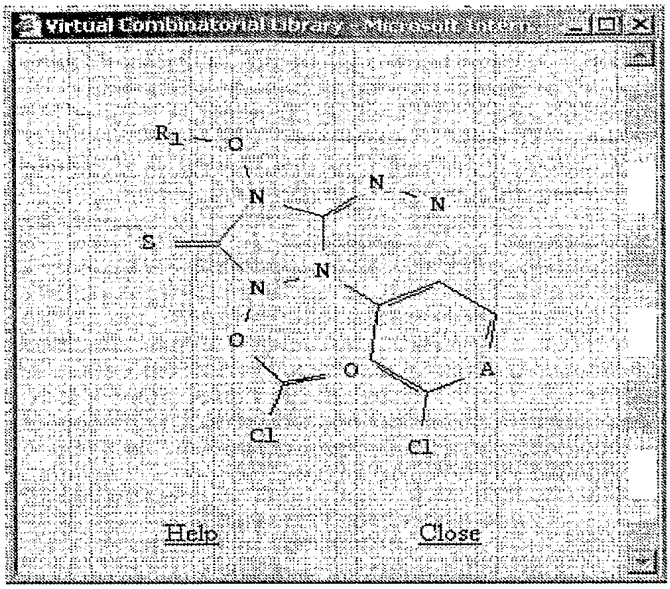

File Edit Insert Format Data Analysis Help
A1
A Structure
B R2
C SUBUBID
D ENTREG
1
R2001
00132_00880_04
00132_00880_04_00001
2
R2003
00132_00880_04
00132_00880_04_00002
3
R2004
00132_00880_04
00132_00880_04_00003
Data Size: 3 rows, 4 columns
No Valid Selection
New data set loaded
0 jobs pending

Figure 19


Virtual Combinatorial Library
R1
O
N
N
N
S
N
N
O
O
A
Cl
Cl
Help
Close